Lower Passaic River Contaminant Fate and Transport (CFT) Model
Documentation for Processors to Generate Bioaccumulation Model Inputs

Post-processors to Extract CFT Model Results

- **Read_rcaf4445_130409.f**: This post-processor extracts results for the layers of the active bed from the global output (RCAF44 and RCAF45).
    - Output Files:
        - **REAF4445_DCHEM.TXT**: Dissolved chemical concentration in sediment porewater (mg/L)
        - **REAF4445_DOC.TXT**: Dissolved organic carbon concentration in sediment porewater (mg/L)
        - **REAF4445_HSED.TXT**: Thickness of layers in the active bed (m)
        - **REAF4445_PCHEM.TXT**: Particulate chemical concentration in sediment (mg/L)
        - **REAF4445_POC.TXT**: Particulate organic carbon concentration in sediment (mg/L)
        - **REAF4445_TCHEM.TXT**: Total chemical concentration in sediment (mg/L)
        - **REAF4445_TSS[1].TXT**: Sediment concentration (mg/L)
- **Read_rcaf1011_140404.f:** This post-processor extracts results for the layers of the water column from the global output (RCAF10 and RCAF11).
    - Output Files:
        - **REAF1011_DCHEM.TXT**: Dissolved chemical concentration (mg/L)
        - **REAF1011_DOC.TXT**: Dissolved organic carbon concentration (mg/L)
        - **REAF1011_PCHEM.TXT**: Particulate chemical concentration (mg/L)
        - **REAF1011_ALGPOC.TXT**: Algal carbon concentration (mg/L)
        - **REAF1011_DETPOC.TXT**: Detrital carbon concentration (mg/L)
        - **REAF1011_TCHEM.TXT**: Total chemical concentration (mg/L)
        - **REAF1011_TSS.TXT**: Total suspended solids concentration (mg/L)
- **Read_rcaf1011_part_140430.f:** This post-processor extracts results for the layers of the water column from the global output (RCAF10 and RCAF11_part)
    - **Output files:**
        - **REAF1011_PCHEM_ALG.TXT**: Particulate chemical concentration associated with Algal carbon (mg/L)
        - **REAF1011_PCHEM_DET.TXT**: Particulate chemical concentration associated with Detrital carbon (mg/L)
- **Read_rcaf6465_layers_140109.f:** This post-processor extracts results for the layers of the archive bed from the global output (RCAF64 and RCAF65).
    - Output Files:

[1] The suffix "_TSS" was applied in the original processor code to refer to sediment bed solids as well (in addition to water column solids), and the naming convention has not been updated subsequently. For sediment bed variables, it is based on the bulk sediment concentration, RCATOX variables SSS1 and SSS2. For water column quantities, it is based on the suspended solids concentration, RCATOX variables SS1 and SS2.

        - **REAF6465OUT.TXT**:
            - Total chemical concentration (mg/L) (5 layers (i.e., layers 11-15) then 15-cm average)
            - Sediment density (mg/L) (5 layers)
            - Particulate organic carbon concentration (mg/L) (5 layers)
            - Thickness of layers in the archive bed (m) (5 layers)
- **Read_rcaf8485_fluff_140121.f:** This post-processor extracts results for the fluff layer from the global output (RCAF84 and RCAF85).
    - Output Files:
        - **REAF8485OUT.TXT**:
            - Total chemical concentration (mg/L)
            - Sediment concentration (mg/L)
            - Particulate organic carbon concentration (mg/L)
            - Dissolved organic carbon concentration (mg/L)
            - Thickness of fluff layer (m)
- The above processors need the file "**ww_cells.txt**" which contains the cell IJ's for all grid cells in the LPR (506).
- To concatenate the individual time chunk text files, use this IDL procedure: **concatenate_timechunks_foodchain_output_txts.pro**
    - Note: This IDL procedure uses the file **"time_eg.txt"**, which contains a list of the individual time-chunks for the corresponding year. An example of this file for year 1011 is included in the transmittal.
- **Read_gcmtran.f:** This post-processor extracts temperature and water surface elevation (WSE) from hydro coupling files (WSE is not currently used).
    - Output File:
        - **TEMPERATURE_YYYY.txt:** Temperature (degrees Celsius)
- **Get_cwcm_waterdepth_v2.f:** This post-processor extracts water depth from the hydro coupling file "gcm_tran" (these are 15-minute averages)
    - This processor also needs "gcm_geom", **"wet_grid"**, and the file **"longmatch_ij.prn"** that contains the cell IJ's for all grid cells.
    - Output File:
        - **Waterdepth_qc.txt:** Water depth (m)
    - Concatenate the individual water depth files to annual files using this IDL procedure: **pascpg_concatenate_waterdepth_chunks.pro**
    - Compute the daily-average water depths using this IDL procedure: **foodchain_waterdepth_txts_compute_daily.pro**

Segment Definition

- The processor generates averages for 26 distinct averaging zones that are referred to as

"Segments".

Segments	Description
1	Sitewide, whole river
2	RM 0-4, whole river
3	RM 4-8.5, whole river
4	RM 8.5-DD, whole river
5	RM 0-2, whole river
6	RM 2-4, whole river
7	RM 8.5-12, whole river
8	RM 12-15, whole river
9	RM 15-DD, whole river
10	RM 12-DD, whole river
11	RM 0-8.5, whole river
12	RM 4-DD, whole river
13	RM 7-DD, whole river
14	Sitewide, mudflat only
15	RM 0-4, mudflat only
16	RM 4-8.5, mudflat only
17	RM 8.5-DD, mudflat only
18	RM 0-2, mudflat only
19	RM 2-4, mudflat only
20	RM 8.5-12, mudflat only
21	RM 12-15, mudflat only
22	RM 15-DD, mudflat only
23	RM 12-DD, mudflat only
24	RM 0-8.5, mudflat only
25	RM 4-DD, mudflat only
26	RM 7-DD, mudflat only

- Segments are identified using a flag stored in the shapefile ***LPR_FDCHN_Segments_rev.shp***
  - Fields H1 and H2 (which are the model grid cell dimensions) and IJ (model grid cell ID's) are used to calculate area-weighted averages
  - Flags for whole river segments are stored in the following shapefile attributes: Flag_WR, Flag_WR2, Flag_WR3, Flag_WR4, Flag_WR5, Flag_WR6, Flag_WR7
  - Flags for mudflat segments are stored in the following shapefile attributes: Flag_MF, Flag_MF2, Flag_MF3, Flag_MF4, Flag_MF5, Flag_MF6, Flag_MF7
  - The flag fields hold different segments since some of them overlap (e.g. Exposure areas 4, 9, and 10)
    - Flag_WR: Whole-river flag; Segment 1
    - Flag_WR2: Whole-river flag; Segment 2-4
    - Flag_WR3: Whole-river flag; Segment 5-9
    - Flag_WR4: Whole-river flag; Segment 10
    - Flag_WR5: Whole-river flag; Segment 11 (flag number 21)

- Flag_WR6: Whole-river flag; Segment 12 (flag number 23)
- Flag_WR7: Whole-river flag; Segment 13 (flag number 24)
- Flag_MF: Mudflats-only flag; Segment 14 (flag number 11)
- Flag_MF2: Mudflats-only flag; Segment 15-17 (flag numbers 12 to 14)
- Flag_MF3: Mudflats-only flag; Segment 18-22 (flag numbers 15 to 19)
- Flag_MF4: Mudflats-only flag; Segment 23 (flag numbers 20)
- Flag_MF5: Mudflats-only flag; Segment 24 (flag number 22)
- Flag_MF6: Mudflats-only flag; Segment 25 (flag number 25)
- Flag_MF7: Mudflats-only flag; Segment 26 (flag number 26)

Processors to Generate Bioaccumulation Model Inputs

- IDL Deck that transforms RCA output to Windward Input: **compile_foodchain_inputs_rev.pro**
  - Year: Model year (integer)
  - Days: Cumulative days in model year (integer)
  - For all variables except Year and Days, there is one column per segment. Segment values are the area-weighted averages of the constituent cells.
    - Water column depth averaging is a straight average because all water column layers have the same thickness (each is 10% of the total water column depth)
    - Sediment depth averaging is depth-weighted average because the top layer of the active bed has a varying thickness. Processor can provide any layer interval average between 1 and 15 layers.
      - The archive bed (layers 11-15) does not have separate output for dissolved and particulate chemical concentration. The partitioning in layer 10 is used to estimate the partitioning in the archive bed.
        - $STCHEM_{10} = SDCHEM_{10} + SPCHEM_{10}$[2]
        - $F_{d,10} = SDCHEM_{10}/STCHEM_{10}$
        - $F_{p,10} = 1 - F_{d,10}$
        - If STCHEM = 0, then $F_{d,10} = F_{p,10} = 0$.
        - $SDCHEM_{Archive} = STCHEM_{Archive} * F_{d,10}$
        - $SPCHEM_{Archive} = STCHEM_{Archive} * F_{p,10}$
  - Occasionally NaN values for TSS are encountered in the CFT output, due to an issue within ECOM-SEDZLJ related to the aggregation of non-cohesive solids when generating the ST-model linkage files[3]. For these outputs, water column CFT model results are not used for the cells with NaN TSS values. This does not affect water temperature or sediment processing.
  - The 1st and last dump for all variables are instantaneous outputs and were excluded

[2] This current formulation is not valid because SDCHEM is computed on a pore volume basis (rather than total sediment volume). However, this does not impact 2-layer processing. The formulation will be updated in the future if needed for averaging below layer 10.

[3] This behavior impacted only non-cohesive solids, and therefore did not propagate through the RCATOX contaminant fate and transport calculations. It was corrected within ECOM-SEDZLJ in mid-2013.

from calculations (the other outputs are time-averaged on a monthly basis)

- This processor generates a text file, which should be pasted into the Windward template.

Variables

- TW (1-26): Water temperature (degrees C)
  - From hydro coupling files
- CWB(1-26): Depth-average bioavailable concentration in water column [ng/g]
  - Equation for calculating this value came from Windward:
  - Filtered water concentration = total dissolved chemical concentration [mg/L] (C_{diss}), sum of truly dissolved and DOC-bound
    - REAF1011_DCHEM.TXT
  - $K_{ow} = 10^{6.81}$ (log K_{ow} = 6.81, from model input file) [L/kg] for 2,3,7,8-TCDD (log K_{ow} = 6.27 for Tetra-CB in model input file).
  - A_{DOC} = 0.0 in this version of the CFT model settings
  - DOC = dissolved organic carbon [mg/L]
    - REAF1011_DOC.TXT
  - Full equation used in IDL:
    - $CWB = (C_{diss}/(1+K_{ow}*A_{DOC}*DOC*10^{-6}))*10^{3}$
    - [ng/g] = ([mg/L]/([.] + [L/kg]*[.]*[mg/L]*[10^{-6} kg/mg]))*[10^{-3} L/ml]*[10^{6} ng/mg]
    - Note: assumes water density of 1 g/cm^3
- CSD(1-26): Depth-average concentration in sediment porewater (ng/g)
  - $CSD = (C_{porewater})*10^{6}$ ng/mg / $Density_{wat}$
    - [ng/g] = [mg/L] * [ng/mg] / [g/L]
    - $Density_{wat} = 10^{3}$ g/L
    - $C_{porewater}$: REAF4445_DCHEM.TXT, REAF6465.TXT
    - $Density_{sed}$: REAF4445_TSS.TXT, REAF6465.TXT
- CST(1-26): Depth-average concentration in sediment solids (ng/g)
  - $CST = (C_{sed}/Density_{sed})*10^{9}$ ng/g
  - [ng/g] = ([mg/L]/[mg/L])*[10^{6} ng/mg]*[10^{3} mg/g]
  - C_{sed}: REAF4445_PCHEM.TXT, REAF6465.TXT
  - $Density_{sed}$: REAF4445_TSS.TXT, REAF6465.TXT
- CPART(1-26): Depth-average concentration in water column detrital particulates (ng/g) [4]
  - $CPART = (C_{wc,part}/TSS)*10^{9}$ ng/g

[4] This formulation is valid for the current CFT model settings as there is no chemical sorption to algal carbon (APHYT=0 in RCATOX). It will be reviewed/updated as needed in conjunction with model calibration refinements.

- [ng/g] = ([mg/L]/[mg/L])*[10^9 ng/g]
- $C_{wc,part}$: REAF1011_PCHEM.TXT
- TSS: REAF1011_TSS.TXT

- CPW(1-26): Depth-average concentration of total suspended solids (kg/L)
  - CPW = TSS/10^6 mg/kg
  - [kg/L] = [mg/L]/[10^6 mg/kg]
- OCSS(1-26): Depth-average organic carbon content of sediment (fraction of total)
  - $OCSS = POC_{sed}/Density_{sed}$
  - [.] = [mg/L] / [mg/L]
  - POC_{sed}: REAF4445_POC.TXT
- OCPART(1-26): Depth-average detrital organic carbon content of water column particulates (fraction of total)
  - $OCPART = POC_{part}/TSS$
  - [.] = [mg/L] / [mg/L]
  - POC_{part}: REAF1011_DETPOC.TXT
  - TSS: REAF1011_TSS.TXT
- CPART_DET(1-26): Concentration in detrital particulates in the BOTTOM LAYER of the water column (ng/g)[4]
  - $CPART\_DET = (C_{wc,part}/TSS)*10^9$ ng/g
  - [ng/g] = ([mg/L]/[mg/L])*[10^9 ng/g]
  - $C_{wc,part}$: REAF1011_PCHEM.TXT
  - TSS: REAF1011_TSS.TXT
- CAC (1-26): Depth-average concentration in algal particulates (ng/g) in water column
  - $CAC = (C_{wc,algal\ part}/POC_{algal\ part})*10^9$ng/g
  - [ng/g] = ([mg/L]/[mg/L))*[10^9 ng/g]
  - $C_{wc,algal\ part}$: REAF1011_PCHEM_ALG.TXT
  - $POC_{algal\ part}$: REAF1011_ALGPOC.TXT
- CAC_DET (1-26): Concentration in algal particulates in the BOTTOM LAYER of the water column (ng/g)
  - $CAC_DET = (C_{wc,algal\ part}/POC_{algal\ part})*10^9$ng/g
  - [ng/g] = ([mg/L]/[mg/L))*[10^9 ng/g]
  - $C_{wc,algal\ part}$: REAF1011_PCHEM_ALG.TXT
  - $POC_{algal\ part}$: REAF1011_ALGPOC.TXT
- OCPart_DET (1-26): Organic carbon content of particulates in the BOTTOM LAYER of the water column (fraction of total)
  - $OCPART\_DET = POC_{part}/TSS$
  - [.] = [mg/L] / [mg/L]
  - POC_{part}: REAF1011_DETPOC.TXT
  - TSS: REAF1011_TSS.TXT
- CST_OCNorm (1-26): Carbon normalized concentration in sediment solids (ng/g)
  - CST_OCNorm = CST/OCSS